LLNL-CONF-417616

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October 6, 2009

2009 International Pittsburgh Coal Conference
Pittsburgh, PA, United States
September 20, 2009 through September 23, 2009

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THERMAL-HYDROLOGICAL SENSITIVITY ANALYSIS OF UNDERGROUND COAL GASIFICATION

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Abstract

This paper presents recent work from an ongoing project at Lawrence Livermore National Laboratory (LLNL) to develop a set of predictive tools for cavity/combustion-zone growth and to gain quantitative understanding of the processes and conditions (natural and engineered) affecting underground coal gasification (UCG). We discuss the application of coupled thermal-hydrologic simulation capabilities required for predicting UCG cavity growth, as well as for predicting potential environmental consequences of UCG operations.

Simulation of UCG cavity evolution involves coupled thermal-hydrological-chemical-mechanical (THCM) processes in the host coal and adjoining rockmass (cap and bedrock). To represent these processes, the NUFT (Nonisothermal Unsaturated-saturated Flow and Transport) code is being customized to address the influence of coal combustion on the heating of the host coal and adjoining rock mass, and the resulting thermal-hydrological response in the host coal/rock. As described in a companion paper (Morris et al. 2009), the ability to model the influence of mechanical processes (spallation and cavity collapse) on UCG cavity evolution is being developed at LLNL with the use of the LDEC (Livermore Distinct Element Code) code. A methodology is also being developed (Morris et al. 2009) to interface the results of the NUFT and LDEC codes to simulate the interaction of mechanical and thermal-hydrological behavior in the host coal/rock, which influences UCG cavity growth.

Conditions in the UCG cavity and combustion zone are strongly influenced by water influx, which is controlled by permeability of the host coal/rock and the difference between hydrostatic and cavity pressure. In this paper, we focus on thermal-hydrological processes, examining the relationship between combustion-driven heat generation, convective and conductive heat flow, and water influx, and examine how the thermal and hydrologic properties of the host coal/rock influence those relationships. Specifically, we conducted a parameter sensitivity analysis of the influence of thermal and hydrological properties of the host coal, caprock, and bedrock on cavity temperature and steam production.

1. Introduction

UCG converts *in situ* coal into a synthesis gas through the same chemical reactions that occur in surface gasifiers. While UCG economics are promising, progress in UCG deployment has been hampered by insufficient modeling methodology and quantitative physical-process understanding. During the 1970s and 1980s, LLNL pioneered the development and application of simulation capability of coupled THCM processes (Britten and Thorsness, 1989) and in conducting field pilot studies of UCG (Stephens, 1981). Since then, we have advanced our simulation capabilities and understanding of THCM processes relevant to UCG and related environmental issues. This paper addresses thermal-hydrological aspects of an ongoing project at LLNL that leverages such advances to develop a simulation capability and understanding of UCG-relevant THCM processes. Our overall goal is to understand how UCG can be engineered to reduce environmental risk, while improving productivity.

The UCG combustion zone occurs in and around a cavity that is partially filled with caved coal rubble (and possibly caprock rubble) from the roof of the cavity (Figure 1). This zone will propagate between injection and production wells. The rate of cavity/combustion-zone growth depends on a number of factors, some of which can be controlled, such as the rate of air and/or air/steam injection, as well as many natural-system factors affected by the THCM properties of the host coal/rock. Host-coal/rock thermal conductivity affects heat conduction. Coal chemistry, oxygen availability, and temperature (controlled by heat-transfer mechanisms) affect combustion and corresponding heat-generation rates. Permeability (particularly within fractures/cleats), along with the difference between hydrostatic and cavity pressure, controls water influx into the combustion zone, the flow of injected and product gas from the cavity into the host coal/rock, the flow of pyrolysis gas from the host coal into the cavity, and convective heat transfer in the host coal/rock. Permeability also affects natural convection that transports heat and aqueous-phase liquids (and contaminants) from the cavity. The ratio of fracture surface area to bulk rock volume affects the potential reaction surfaces for combustion. Geomechanical properties of the fractures and coal/rock matrix affect the stability and caving of roof materials. Fracture properties will change as combustion proceeds. All of these effects will interact in a highly dynamic, non-linear manner, influencing the growth of the coal cavity within a heterogeneous host-coal/rock environment.

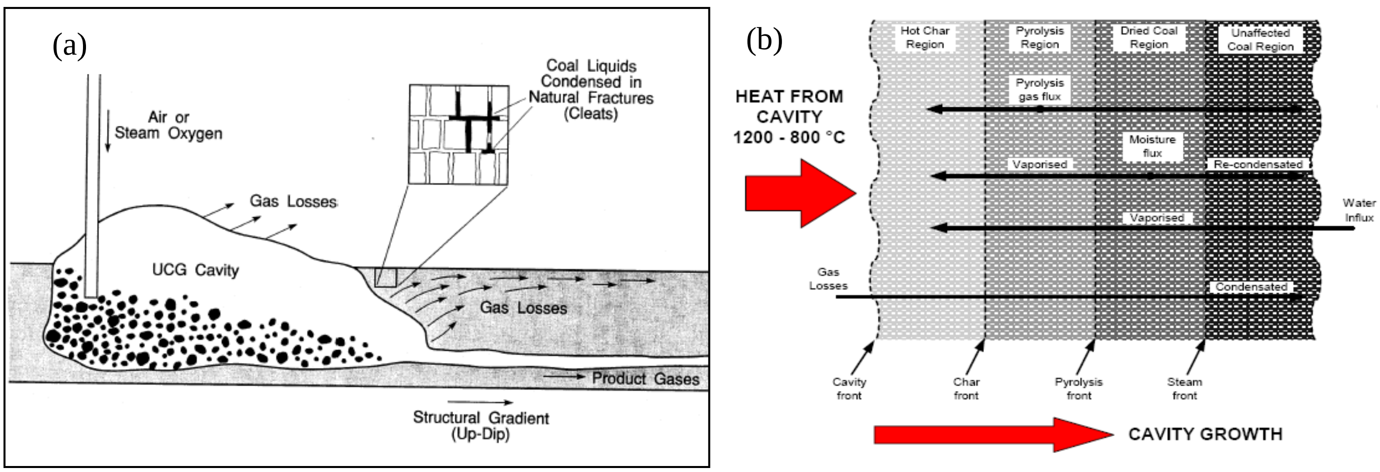


Figure 1. Schematics of the UCG cavity growth process (a) and cavity side wall (b) are shown. Panel (a) is from Covell and Thomas (1996). Panel (b) is from www.berr.gov.uk (2008).

2. Modeling Thermal-Hydrological Behavior

Multi-phase (gas and liquid) fluid flow and heat transfer in the host coal/rock occurs in fractures/cleats and in the porous coal/rock matrix. Matrix porosity (micropores) contains the majority of the coal/rock porosity and stored fluids, while fracture/cleat porosity (macropores) provides the primary conduits for large-scale fluid flow and convective heat transfer (Figure 2). Fracture-matrix flow interaction can be represented by different conceptual/numerical models: (1) discrete-fracture models, which are computationally expensive and generally impractical for large-scale applications, and (2) dual-continuum models, often called dual-porosity/permeability models (DKM), which represent the matrix and fracture porosity as overlapping interacting continua with mass and heat transfer between the fracture and matrix continua. We apply the DKM to the NUFT code to represent fracture-matrix interaction in the host coal/rock. NUFT, which runs on massively-parallel platforms, simulates multiphase, multi-component heat and mass flow and reactive transport in unsaturated and saturated porous media (Nitao, 1998). NUFT has been used to solve complex problems in nuclear waste management (Buscheck et al. 2002, 2003a, 2003b), environmental remediation, and CO_2 sequestration (Carroll et al. 2009). In addition to simulating the thermal-hydrological response of the coal/rock environment, NUFT can be used to simulate the transport and fate of injected and product gases and liquid-phase byproducts of the UCG reactions, as well as CO_2 sequestration in the coal cavity after UCG operations have been completed.

Thermal conditions in the UCG cavity are strongly influenced by water influx, which is controlled by the permeability distribution in the host coal and adjoining rock layers and the difference between hydrostatic and cavity pressure. Figures 3a and 3b illustrate this dependence. A radially-symmetric model of a UCG cavity is used to represent a 0.2-m-diameter by 10-m-long (horizontally-oriented) cavity/combustion zone. The model represents the production well as a specified pressure sink and the influence of coal combustion is represented with a specified heat-generation rate of 13 kW for 100 days. The influence of thermal radiation in the cavity is represented by assigning a large value of thermal conductivity to the cavity.

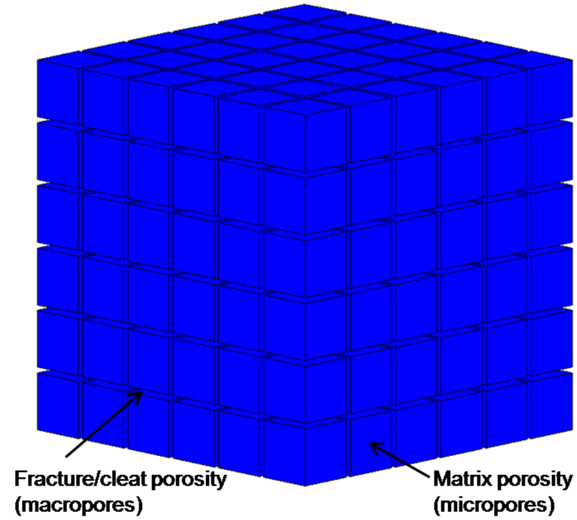


Figure 2. Schematic of the dual-continuum model is shown, including the fracture continuum, representing the fracture/cleat porosity (macropores) and the matrix continuum, representing the matrix porosity (micropores).

Figure 3a shows the sensitivity of cavity temperature to coal cleat permeability, ranging between 1 and 10 millidarcy (md). Figure 3b shows the sensitivity of cavity temperature to cavity underpressure, which is defined to be the difference between the hydrostatic pressure in the coal and the cavity pressure. Cavity temperature responds to relative changes in coal cleat permeability in the same fashion that it responds to relative changes in cavity underpressure. Water influx, which is linearly dependent on the product of coal cleat permeability and cavity underpressure, has a strong cooling effect by virtue of phase change (boiling) in the coal and the convection of latent heat, as steam flows into the cavity and along the axis of the cavity towards the production well, where it leaves the host coal/rock environment. Note that if the gasification reactions (reforming, water gas shift, and methanation) were represented in this model, some of this loss of latent heat would occur with the flow of product gases (H_2, CO, CO_2, and CH_4) out of the production well.

The influence of coal-cleat-permeability heterogeneity on cavity temperature is shown in Figure 3c, which compares a heterogeneous case with 1 and 10 md cleat permeability zones with homogeneous cases with cleat permeabilities of 5 and 6 md. Cavity temperature for the heterogeneous case, which has an average cleat permeability of 5.5 md, lies between the cavity temperatures for the 5 and 6 md cases. The influence of thermal radiation and convection within the cavity homogenizes cavity temperature, which has the effect of averaging the influence of heterogeneous water influx towards the cavity/combustion zone. Thus, the total influx of water into the cavity/combustion zone determines the overall convective cooling effect on cavity temperature.

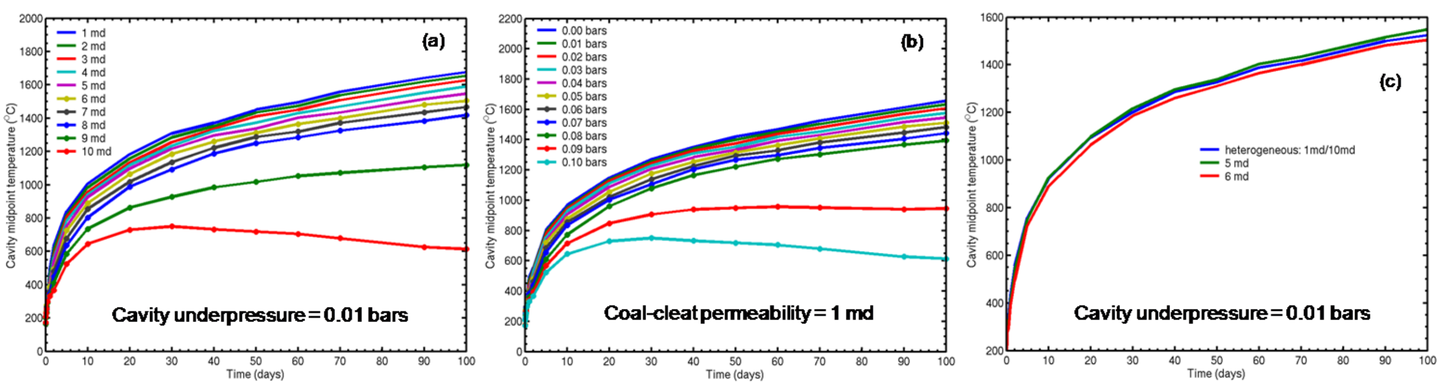


Figure 3. Cavity temperature sensitivity to (a) coal cleat permeability and (b) cavity underpressure (hydrostatic – cavity pressure) are shown. (c) Cavity temperature for a heterogeneous case with average cleat permeability of 5.5 millidarcy (md) is compared with those of homogeneous cases with cleat permeabilities of 5 and 6 md. Plotted cavity temperatures correspond to the center of a 0.2-m-diameter by 10-m-long cavity/combustion zone, with a heat-generation rate of 13 kW.

3. Analysis of Thermal-Hydrological Behavior for Hoe Creek III Pilot Test

During the late 1970s, LLNL conducted three *in situ* UCG pilot tests at the Hoe Creek site in Wyoming (Stephens, 1981). The stratigraphic sequence at Hoe Creek consists of sandstones, claystones, and Felix No.1 and 2 coal seams, with Felix No.2 coal seam being the target for the pilot tests. The hydrostratigraphic sequence applied in the 3-D thermal-hydrologic model (Figure 4) used in this study is a slight simplification of the stratigraphic sequence reported by Covell and Thomas (1996). Permeabilities are based on data from Stone et al (1983). The Felix No.1 and 2 coal seams are assigned horizontal and vertical coal cleat permeabilities of 230 and 23 md, respectively; the caprock units are assigned horizontal and vertical fracture permeabilities of 120 and 22 md, respectively; and the bedrock is assigned an isotropic fracture permeability of 1 md. The matrix permeability of all units is assumed to be 0.01 md. We simulated the first 5 days of the third pilot test (Hoe Creek III), during which time air was injected at a rate of 0.96 kg/sec. The model approximates the average shape of the cavity during the first 5 days, and the heating effect of combustion is approximated with a constant heat-generation rate of 1200 kW. Figure 5 plots temperature and the distribution of liquid-phase saturation and pressure change, relative to ambient pressure, in the fracture continuum. The extraction of steam in the production well causes a sink that draws water influx from a wide region of the groundwater system, causing a pressure perturbation felt at the water table within the first 4 hours of the test (Figure 5b).

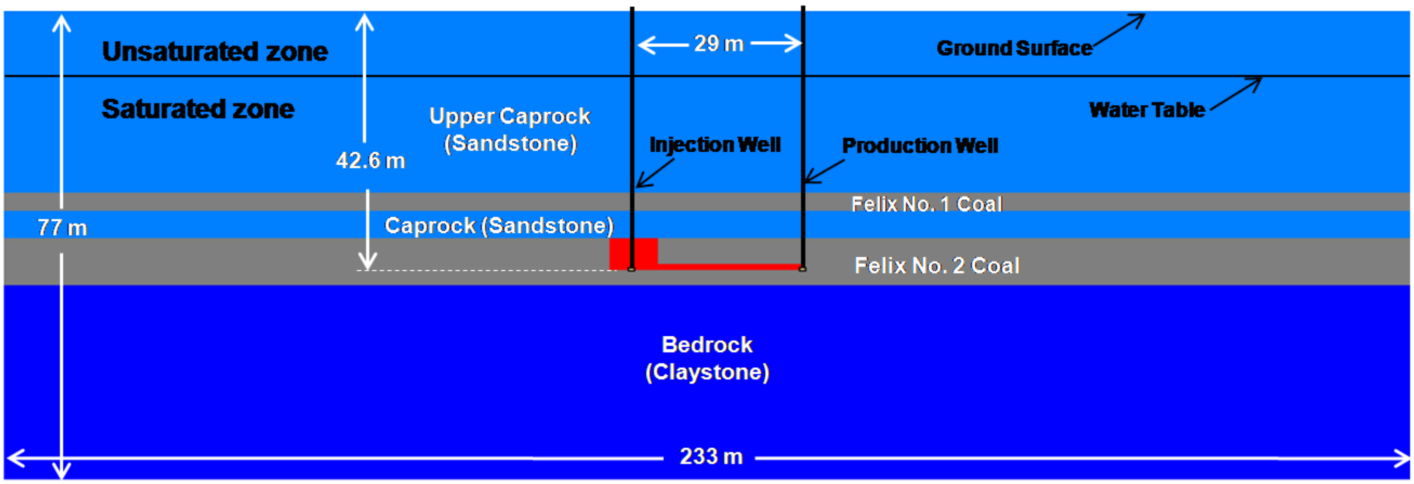


Figure 4. The hydrostratigraphic sequence applied in the 3-D thermal-hydrological model of the Hoe Creek III UCG pilot study is shown. The model extends 300 m in the lateral direction (orthogonal to the cavity axis).

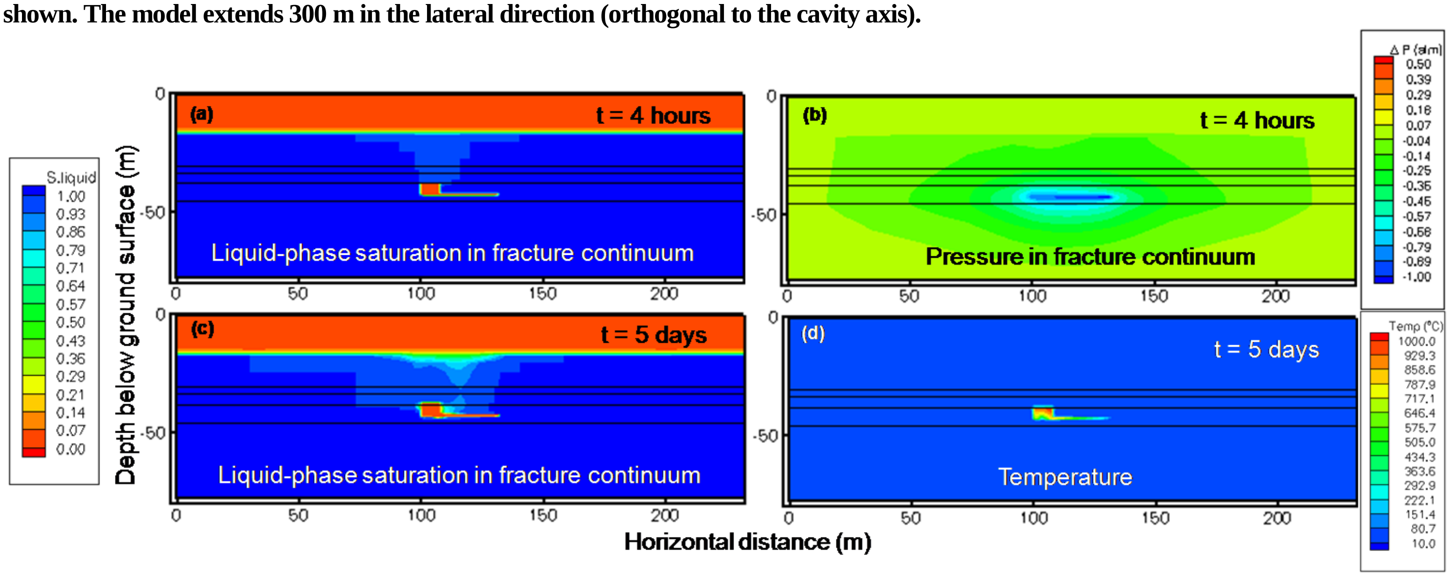


Figure 5. Liquid-phase saturation (a) and pressure change (b), relative to ambient pressure, in the fracture continuum are plotted 4 hours after the start of the test. Liquid-phase saturation in the fracture continuum (c) and temperature (d) are plotted at 5 days.

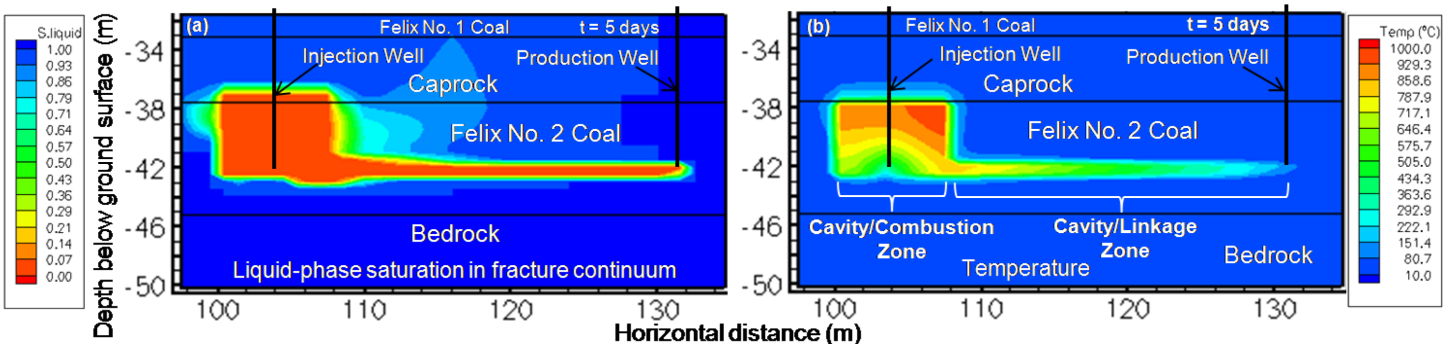


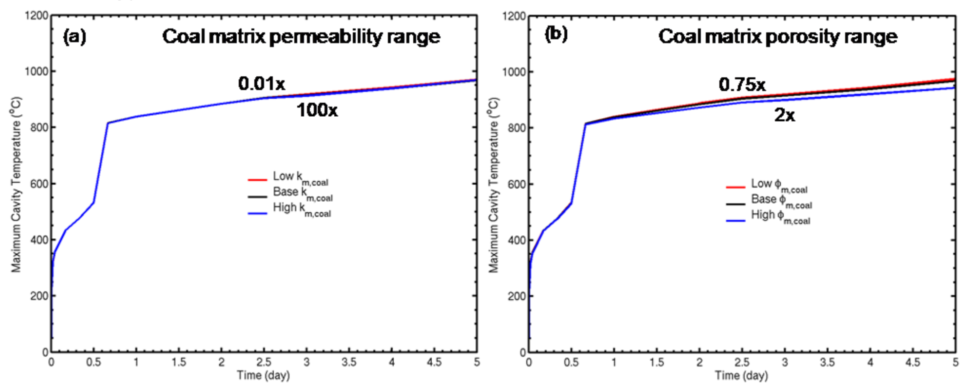
Figure 6. Liquid-phase saturation in the fracture continuum (a) and temperature (b) is plotted 5 days after the start of the test.

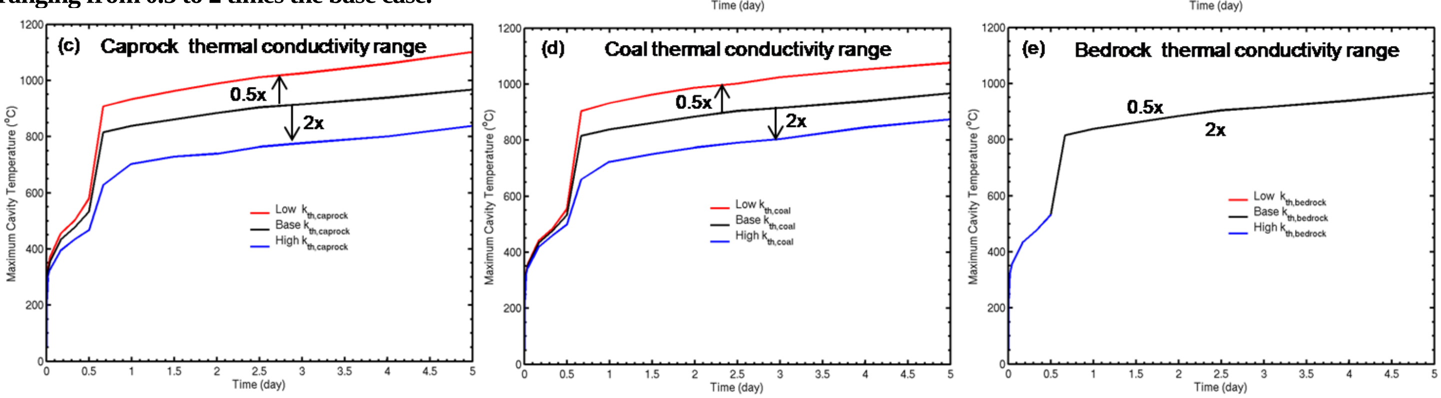
The distributions of temperature (Figure 6b) and liquid-phase saturation in the fracture continuum (Figure 6a) are plotted in the vicinity of the cavity/combustion zone and cavity/linkage zone 5 days after the start of combustion. Note that the cavity/linkage zone is the conduit for product gases from the cavity/combustion zone to the production well. The temperature distribution in and around the cavity/combustion zone (Figure 6b) shows that the thermal perturbation has propagated about a meter away from the cavity and into the coal and overlying caprock. The liquid-phase saturation distribution (Figure 6a) shows that partial dryout has also propagated about a meter away from the cavity into the caprock and somewhat further into portions of the coal. The temperature distribution in the cavity/combustion zone (Figure 6b) shows the influence of buoyant gas-phase convection and the cooling effect of air injection at the bottom of the cavity. The temperature distribution in the cavity/linkage zone (Figure 6b) shows the influence of convective latent heat transfer all the way to the production well.

3.1 Influence of Coal Matrix Permeability and Porosity

Cavity temperature is found to be insensitive to coal matrix permeability over a four order of magnitude range of matrix permeability (Figure 7a), as well as being insensitive to coal matrix porosity (Figure 7b). Because large-scale flow of water primarily occurs through fractures and cleats, the majority of water influx towards the cavity/combustion zone occurs through fractures and cleats; consequently matrix permeability has a negligible influence on the rate of water influx. The energy required to drive (vaporize) *in situ* water from matrix pores is

Figure 7. Maximum cavity temperature history is plotted for a range of hydrologic and thermal properties, including (a) coal matrix permeability, ranging from 0.01 to 100 times the base-case value, (b) coal matrix porosity, ranging from 0.75 to 2 times the base case, (c) caprock thermal conductivity, ranging from 0.5 to 2 times the base case, (d) coal thermal conductivity, ranging from 0.5 to 2 times the base case, and (e) bedrock thermal conductivity, ranging from 0.5 to 2 times the base case.





negligible compared to that required to vaporize water influx through fractures and cleats; consequently, matrix porosity has a negligible influence on thermal behavior near the cavity/combustion zone. Because matrix permeability and porosity in the coal have a negligible influence on cavity temperature, it is expected that matrix permeability and porosity in the caprock and bedrock also have a negligible influence on temperature.

3.2 Influence of Thermal Conductivity in the Caprock, Coal, and Bedrock

Cavity temperature is seen to be moderately sensitive to thermal conductivity in the caprock and coal (Figure 7c and d). As evident in Figure 6b, buoyant gas-phase convection exerts a strong influence on the cavity temperature distribution; notably, by steepening the thermal gradient at the top of the cavity. This steepened thermal gradient enhances heat loss to the caprock; consequently, caprock thermal conductivity has a slightly stronger influence on cavity temperature than coal thermal conductivity, as is evidenced by comparing Figures 7c and 7d. Because the thermal front does not reach the bedrock during the first 5 days of the Hoe Creek III pilot test, and because the thermal gradient is less steep at the bottom of the cavity, thermal conductivity in the bedrock does not influence cavity temperature (Figure 7e).

3.3 Influence of Caprock and Bedrock Fracture Permeability and Coal Cleat Permeability

In general, cavity temperatures are found to be strongly affected by fracture and cleat permeability (Figure 8). Cavity temperature is most sensitive to coal cleat permeability, followed by bedrock and caprock fracture permeability. The driving force for water influx towards the cavity/combustion zone is the difference between and hydrostatic and cavity pressure, which is greater below the cavity than above the cavity. Because of the strong sensitivity of cavity temperature to the magnitude of water influx, cavity temperature is more sensitive to fracture permeability in the bedrock than in the caprock. For all the thermal and hydrological properties investigated, fracture/cleat permeability is found to have the greatest influence on temperature.

While cavity temperature is found to be very sensitive to fracture/cleat permeability, it is useful to consider that sensitivity in terms of heat-generation rate. Figure 9 shows the increase in heat-generation rate required to accommodate an increase in fracture/cleat permeability to achieve the same cavity temperature. For a factor of 2 increase in coal cleat permeability (Figure 9a), increasing the heat-generation rate by 21.7% achieves the same cavity temperature. If coal combustion is rate limited by the availability of oxygen, this increase in heat-generation rate could be achieved by a 21.7% increase in air injection rate. For a factor of 2 increase in caprock fracture permeability (Figure 9b), increasing the heat-generation rate by 2.5% achieves the same cavity temperature. Because cavity pressure exceeds hydrostatic pressure in the caprock, the heat-generation rate required to maintain a target cavity temperature is much less sensitive to caprock fracture permeability than to coal cleat permeability. For factors of 220/22 increase in bedrock horizontal/vertical fracture permeability (Figure 9c), increasing the heat-generation rate by 10% achieves the same cavity temperature. For factors of 440/44 increase in bedrock horizontal/vertical fracture permeability (Figure 9d), increasing the heat-generation rate by 16.7% achieves the same cavity temperature.

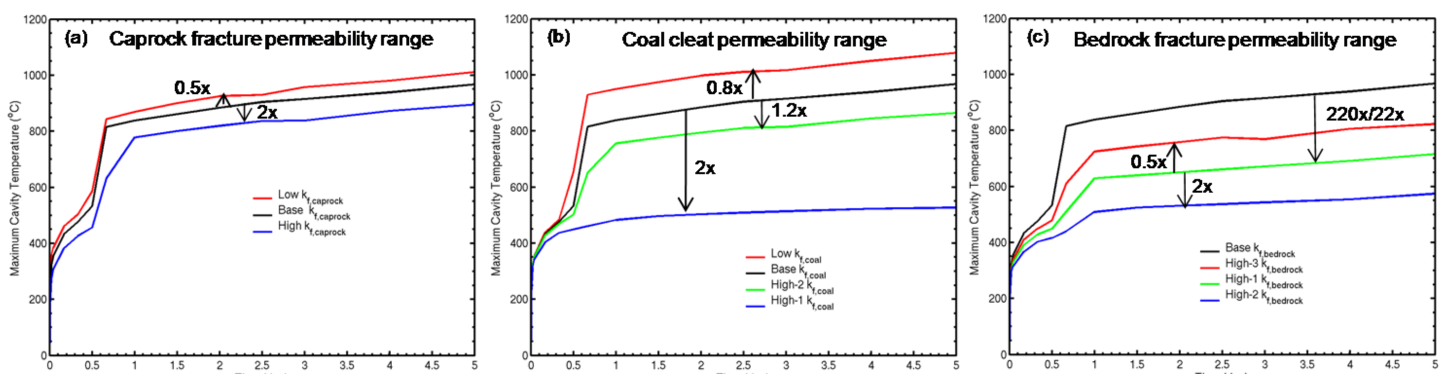
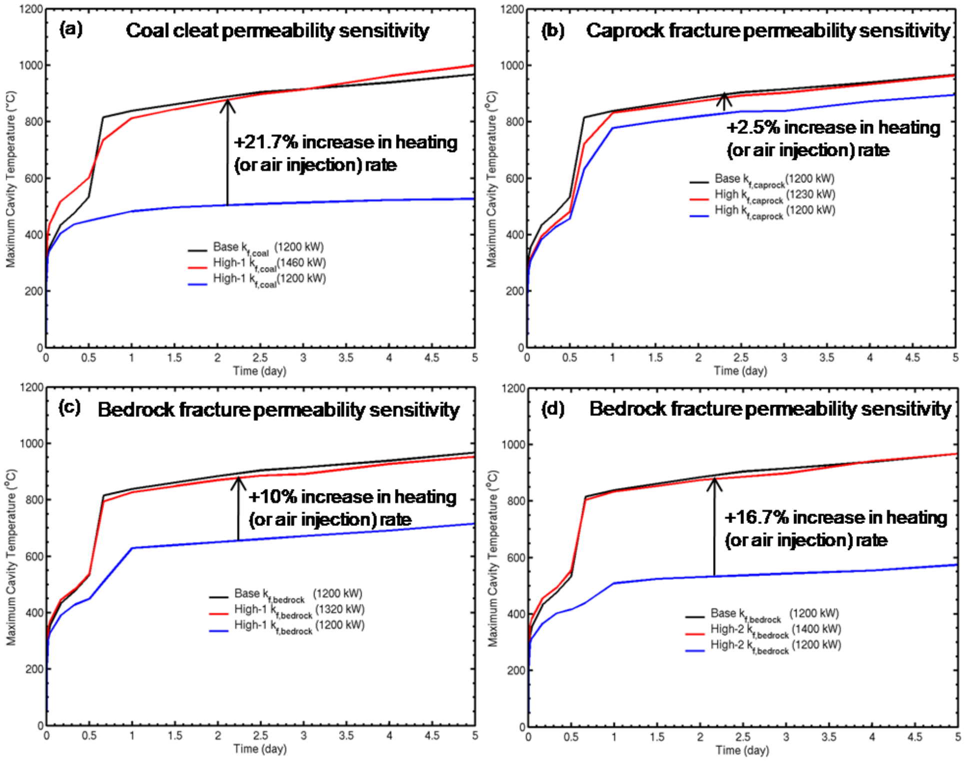


Figure 8. Maximum cavity temperature history is plotted for a range of fracture/cleat permeabilities, including (a) caprock fracture permeability, ranging from 0.5 to 2 times the base-case value, (b) coal cleat permeability, ranging from 0.8 to 2 times the base-case value, and (c) bedrock fracture permeability, with horizontal permeability ranging from 110 to 440 times the base-case value and vertical permeability ranging from 11 to 44 times the base-case value. A heat-generation rate of 1200 kW is applied in these cases.

Figure 9. The increase in heat-generation rate required to accommodate an increase in fracture/cleat permeability to achieve the same cavity temperature is shown for (a) factor of 2 increase in coal cleat permeability, (b) factor of 2 increase in caprock fracture permeability, (c) factors of 220/22 increase in bedrock horizontal/ vertical fracture permeability, and (d) factors of 440/44 increase in bedrock horizontal/vertical fracture permeability.



Factor of two change in fracture/cleat permeability	Percentage change in heating rate to accommodate permeability change
Caprock	2.5%
Coal	21.7%
Bedrock	6.1%

Table 1. The information from Figure 9 is summarized.

Table 1 summarizes the information from Figure 9. Note that the 6.1% increase in heat-generation rate required to achieve the same cavity temperature for a factor of 2 increase in bedrock fracture permeability is obtained by comparing the respective heat-generation rates in Figure 9c (1320) kW and Figure 9d (1400 kW). While cavity temperature is sensitive to fracture/cleat permeability, a target temperature can be attained with relatively minor adjustments to heating (or air injection) rates, which has implications on UCG design and operations.

3.4 Sensitivity of Steam Production to Fracture/Cleat Permeability

Figures 10 and 11 plot the steam production rates for the fracture/cleat permeability sensitivity cases addressed in the previous section (Section 3.3). For early time, steam production is insensitive to fracture/cleat permeability (Figure 10) because that steam production is derived from boiling *in situ* water from the matrix continuum (micropores). For later time, steam production increases with fracture/cleat permeability because that steam production is derived from the boiling of the influx of water that occurs within the fracture/cleat continuum (macropores). Figure 11 shows that steam production increases linearly with heat-generation rate.

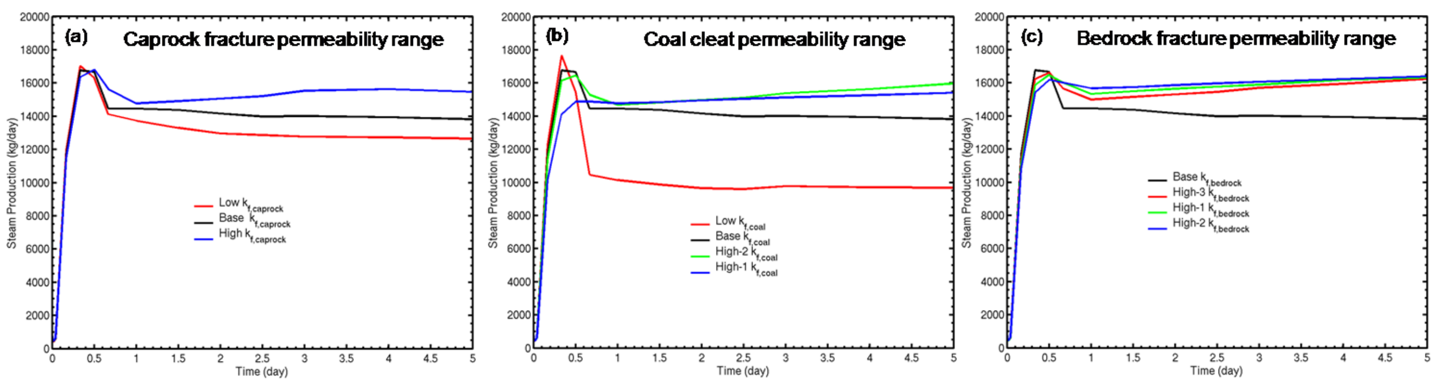


Figure 10. Steam production rate (kg/day) is plotted for a range of fracture/cleat permeabilities, including (a) caprock fracture permeability, ranging from 0.5 to 2 times the base-case value, (b) coal cleat permeability, ranging from 0.8 to 2 times the base-case value, and (c) bedrock fracture permeability, with horizontal permeability ranging from 110 to 440 times the base-case value and vertical permeability ranging from 11 to 44 times the base-case value. A heat-generation rate of 1200 kW is applied in these cases.

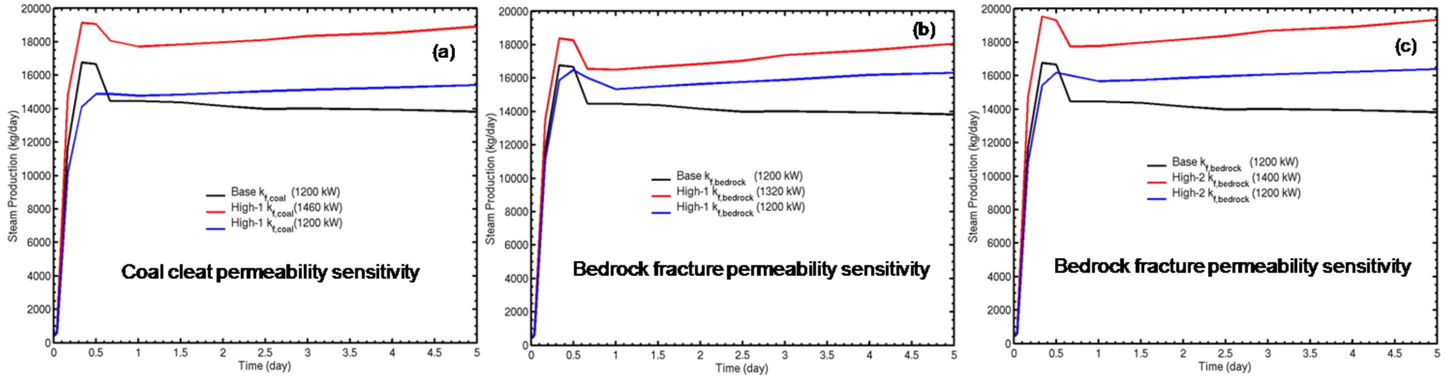


Figure 11. Steam production rate (kg/day) is plotted for the cases plotted in Figure 9, with panel (a) corresponding to Figure 9a, panel (b) corresponding to Figure 9c, and panel (c) corresponding to Figure 9d.

4. Summary and Conclusions

We conducted a parameter sensitivity study of thermal-hydrological behavior of UCG, using the NUFT code. Cavity temperature is found to be strongly influenced by water influx to the cavity/combustion zone, controlled by fracture/cleat permeability and the difference between hydrostatic and cavity pressure. A sensitivity study of the Hoe Creek III UCG pilot test showed that the extraction of steam in the production well caused a sink that drew water influx from a wide region of the aquifer system, with the pressure perturbation being felt at the water table within hours of the start of combustion. Cavity temperature and steam production rate are found to be (1) insensitive to coal matrix permeability and porosity and to bedrock thermal conductivity, (2) moderately sensitive to caprock and coal thermal conductivity, and (3) most sensitive to coal cleat permeability, followed by bedrock and caprock fracture permeability. The influence of fracture/cleat permeability on cavity conditions can be accommodated by adjusting the heating (or air injection) rate.

5. Disclaimer

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. We acknowledge the helpful review comments from Jim Blink.

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